

## Comparative Study of the Water Response to External Force at Nanoscale and Mesoscale

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**Abstract:** Dissipative particle dynamics (DPD) and molecular dynamics (MD) are both Lagrangian particle-based methods with similar equations except that the DPD specification for the force definition on the particles is the result of coarse-graining, and these two methods usually get the similar results in some specific cases. However, there are still some unknown differences between them. Considering the water response to external force, a comparative study of DPD and MD is conducted in this paper, which provides a better understanding on their relation, and a potential way to effectively bridge nanoscale and mesoscale simulation procedures. It is shown that there is a scale effect on the water response to external force between MD and DPD, and that the size effect exists only in MD simulations.

**Keywords:** Dissipative particle dynamics (DPD), molecular dynamics (MD), water response, scale and size effects.

### 1 Introduction

Molecular dynamics (MD) simulation is a powerful technique that has been proved to be able to produce realistic results in a wide variety of applications [Alder and Wainwright (1957); Atluri and Srivastava (2002); among others]. But it becomes inefficient and even impractical beyond extremely small spatial and temporal scales [Klein and Shinoda (2008); Ma, Lu, Wang and Hornung (2006); Tang, Guo and Gao (2011); among others]. When it comes to larger scale, especially when one is concerned with the scale more relevant to biological processes, the

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so-called mesoscopic (between the molecular and continuum scales) methods are the way to go [Hoogerbrugge and Koelman (1992); Liu and Liu (2003); among others]. Obviously, many interesting processes occur at a variety of scales spanning from atomistic length-scale to macroscopic world. Thus, several types of multiscale models have been proposed to combine or couple the molecular method with the numerical procedures at a larger scale, such as dissipative particle dynamics (DPD) [Mukhopadhyay and Abraham (2009)], the multiscale material point method (MPM) [Chen, Han, Jiang, Gan and Sewell (2012)] and Eulerian continuum-based Navier-Stokes equations [Yasuda and Yamamoto (2008)]. Although many efforts have been made in the past, the connection from atomistic scale to macroscopic scale is still not well-understood.

Mukhopadhyay and Abraham (2009) proposed a multiscale model based on the combination of the DPD at mesoscale with the MD at nanoscale, which was used to solve Poiseuille and Couette flows and the flow over a rough wall. They employed the isothermal compressibility of the system to provide a link between the nanoscale and mesoscale description of fluid flow, but the characteristics of compression were not mentioned. Chen, Han, Jiang, Gan and Sewell (2012) presented a particle-based multiscale simulation procedure for establishing the multiscale equation of state (EoS), in which MD at nanoscale is linked with cluster dynamics (CD) at sub-micron scale via a hierarchical approach while CD is embedded into the MPM via a concurrent approach. In the multiscale method combining the MD with Eulerian continuum-based Navier-Stokes equations, MD is coupled with a finite-discretization solver to solve the continuum equations [Connell and Thompson (1995); Voulgarakis and Chu (2009)]. However, a detailed comparative study of the responses at different scales has not been performed in the previous investigations.

Groot and Warren (1997) first made a link between the DPD parameters and  $\chi$ -parameters in the Flory-Huggins type of models that bridged the gap between microscopic and mesoscopic simulations. However, the solutions obtained with the DPD soft repulsion model differ from those with the Flory-Huggins model. On the other hand, the DPD parameters were calibrated based on the analogy of specific macroscopic property so that they might not be consistent with the actual conditions in general. To clarify the size effect on the solutions obtained at different scales, a comparative study between the MD and DPD simulations of the water response to external force is therefore performed in this paper.

## 2 Particle-based simulation techniques

MD has been discussed extensively since the seminal papers of Alder (1957), Gibson (1960) and Rahman (1964) were published. The dynamics of a system with a

certain amount of atoms is obtained by the numerical integration of the equation of motion for each atom as follows:

$$m_i \frac{\partial^2 \mathbf{r}_i}{\partial t^2} = - \frac{\partial}{\partial \mathbf{r}_i} U_{tot}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N), i = 1, 2, \dots, N \quad (1)$$

where,  $m_i$  and  $r_i$  are respectively the mass and position vector of atoms  $i$ ,  $U_{tot}$  is the total potential energy that depends on all the atomic positions and is divided into two parts, namely, nonbonded atom interaction and intramolecular interaction.

The Lennard-Jones potential is a widely used form for simple non-bonded interaction fluids, and given by

$$U_{vdW}(r_{ij}) = 4\epsilon [c_{ij}(\frac{\sigma}{r_{ij}})^{12} - d_{ij}(\frac{\sigma}{r_{ij}})^6] \quad (2)$$

where  $\epsilon$  is the depth of the potential well,  $\sigma$  is the separation distance at which this potential becomes zero,  $r_{ij}$  is the distance between atoms  $i$  and  $j$ , and  $c_{ij}$  and  $d_{ij}$  are dimensionless constants. The interaction occurs within the a certain cutoff distance  $r_c$ . Based on Banerjee's (2007) sensitivity analysis, the cutoff distance in our study is taken to be 9.8 Å.

Another non-bonded potential is the electrostatic potential expressed by the Coulomb's law:

$$U_{coulomb}(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \quad (3)$$

where  $q_i$  and  $q_j$  are respectively the electrostatic charges of atoms  $i$  and  $j$ , which are equal to 0.41 for H atom and -0.82 for O atom, and  $\epsilon_0$  is the dielectric constant. The intramolecular interaction in our study is based on the following approximation:

$$U_{intramolecular} = U_{stretch} + U_{angle} \quad (4)$$

where  $U_{stretch}$  describes the potential when the bond is stretched from its initial position  $r_0$  to a new position  $r$ ,

$$U_{stretch} = k_{bond}(r - r_0)^2 \quad (5)$$

and  $U_{angle}$  describes the potential when the angle between two specific bonds shifts from its initial angle  $\theta_0$  to a new angle  $\theta$ , i.e.,

$$U_{angle} = k_{angle}(\theta - \theta_0)^2 \quad (6)$$

Other intramolecular potential functions such as dihedral and improper dihedral potential functions are not considered here because such a possibility does not appear in our study.

Designed conceptually by Hoogerbrugge (1992), the interactions in DPD model are formulated based on MD by coarse-graining the details at the molecular level to capture the essential feature of physics at the mesoscale. DPD has been developed to simulate complex fluid flows and colloidal phenomena in mesoscopic scale. The motion of a set of interacting “particles” instead of atoms is simulated by the DPD method, in which the particles move according to Newton’s second law, namely

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{v}_i}{dt} = \sum_j \mathbf{f}_{ij} \quad (7)$$

where  $r_i$  and  $v_i$  are respectively the position and velocity vector of the mass centre of particle  $i$ . The particle mass is taken as the unit of mass for convenience.  $\mathbf{f}_{ij}$  is the interparticle force on particle  $i$  by particle  $j$ , which is assumed to be pairwise additive and consists of three parts: a conservative force  $\mathbf{f}_{ij}^C$ , a dissipative force  $\mathbf{f}_{ij}^D$  and a random force  $\mathbf{f}_{ij}^R$ , i.e.,

$$\mathbf{f}_{ij} = \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R \quad (8)$$

In Eq. (7), the summation runs over all other particles around particle  $i$  within a certain cutoff radius  $r_c$ , taken as the unit of length in the conventional DPD formulation. The value of  $r_c$  can be different for different types of forces. The conservative force  $\mathbf{f}_{ij}^C$  is a soft repulsion and given by

$$\mathbf{F}_{ij}^C = \begin{cases} a_{ij}(1 - r_{ij}) \hat{\mathbf{r}}_{ij}, & r_{ij} < 1.0 \\ 0, & r_{ij} \geq 1.0 \end{cases} \quad (9)$$

where  $a_{ij}$  is a maximum repulsion between particles  $i$  and  $j$ . In the current study, the cutoff radius for the conservative force is set to be 1.0, as the unit of length;  $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ , with its amplitude  $r_{ij} = |\mathbf{r}_{ij}|$ , and  $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/r_{ij}$  is the unit vector directed from the mass centre of particle  $j$  to  $i$ . The dissipative and random forces take the form of

$$\mathbf{F}_{ij}^D = -\gamma w^D(r_{ij}) (\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij}) \hat{\mathbf{r}}_{ij} \quad (10)$$

and

$$\mathbf{F}_{ij}^R = \sigma \zeta_{ij} w^R(r_{ij}) \hat{\mathbf{r}}_{ij} \quad (11)$$

respectively, where  $\gamma$  and  $\sigma$  are the coefficients for characterizing the strengths of these forces.  $w^D(r_{ij})$  and  $w^R(r_{ij})$  are  $r$ -dependent weighting functions vanishing

for  $r > r_c$ . Also,  $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ , and  $\zeta_{ij}$  is Wiener increment with the following properties:

$$\langle \zeta(t)_{ij} \rangle = 0 \quad \text{and} \quad \langle \zeta_{ik}(t) \zeta_{jl}(t') \rangle = (\delta_{ij} \delta_{kl} + \delta_{il} \delta_{jk}) \delta(t - t'), \quad (12)$$

in which  $i \neq k$  and  $j \neq l$ . The detailed balance condition is similar to the Fluctuation-Dissipation theorem with the relation between the strength of the random force and the mobility of a Brownian particle, which requires that

$$w^D(r) = [w^R(r)]^2, \quad \gamma = \frac{\sigma^2}{2k_B T} \quad (13)$$

where  $k_B$  is the Boltzmann constant and  $T$  is the temperature of the system. This ensures that the particulate temperature, strictly speaking, the fluctuation kinetic energy of the system, remains in constant. As far as the thermal energy is concerned, the random two-particle force  $\mathbf{F}_{ij}^R$  represents the results of thermal motion of all atoms/molecules contained in particles  $i$  and  $j$ , “heating up” the system. The dissipative force  $\mathbf{F}_{ij}^D$  reduces the relative velocity of two particles and removes kinetic energy from their mass centre to cool the system down. When Eq. (13) is satisfied, the system temperature will approach the given value. The dissipative and random forces act like a thermostat in the conventional molecular dynamics (MD) system.

### 3 Methodology

Water is probably the most common material which has been studied widely in the past. In the MD method, many “hypothetical” models, e.g. SPC, SPC/E, TIP3P, TIP4P and TIM2-F, have been proposed. The effects of those models on certain properties of water, such as density, enthalpy of vaporization, radial distribution function (RDF) and hydrogen bonding have also been investigated extensively [Alexiadis and Kassinos (2008); among others]. However, some of its characteristics and properties have not been clearly defined yet. In this study, three commonly used models, SPC/E [Berendsen, Grigera and Straatsma (1987)], TIP3P [Jorgensen and Chandrasekhar (1983)] and TIP4P [Mahoney and Jorgensen (2000)] are selected with the parameters described in Tab. 1.

Six hundred atoms, four hundred bonds and two hundred angles for each model are created using Packmol [Martinez and Andrade (2009)] and displayed by VMD [Humphrey, Dalke and Schulten (1996)] (Fig. 1). The MD simulations are carried out by utilizing LAMMPS [Plimpton (1995)] with the initial velocities of Maxwellian distribution for molecules at an average temperature 298K, while a Nose-Hoover [Nose (1984), Hoover(1985)] thermostat is utilized to keep the system at 298K during the simulation.

Table 1: Parameters of three water models

Model	$\sigma_{o-o}(\text{\AA})$	$\epsilon_{0-0}(\text{kJ mol}^{-1})$	$r_0(r_1)(\text{\AA})$	$q_H(e)$	$q_O(e)$	$\theta_0(\text{deg})$
<i>SPC/E</i>	3.166	0.650	1.0	+0.4238	-0.8476	109.47
<i>TIP3</i>	3.15061	0.6364	0.9572	+0.4170	-0.8340	104.52
<i>TIP4P</i>	3.15365	0.6480	0.9572	+0.52	-1.04	104.52

$\sigma_{o-o}$  and  $\epsilon_{0-0}$  are the Lennard-Jones parameters for the oxygen-oxygen interaction,  $r_0(r_1)$  is the  $O-H$  bond distance,  $q_H$  and  $q_O$  are the partial charges located respectively on the hydrogen and the oxygen, and  $\theta_0$  is the  $H-O-H$  bonds angle.

The DPD parameters should be carefully chosen so that the water flow could be simulated. Groot and Warren (1997) found that, to satisfy the compressibility of water, the coefficient of the conservation force should be

$$a_{ij} = 75k_B T / \rho \quad (14)$$

and recommended that  $\sigma=3.0$  with  $\lambda=0.65$  in the Verlet-type algorithm. The density is set to be  $\rho=4.0$ . The size of the plane lattice of the wall particles is equal to 1.0. The unit of energy is set to be  $k_B T$ , i.e.,  $k_B T=1.0$ . According to Eq. (13),  $\gamma=4.5$ . From Eq. (14),  $a_{ij} = a_{ff}=18.75$ . We assume that  $a_{ww}=5.0$  and  $a_{fw} = \sqrt{a_{ff}a_{ww}}=9.6825$  when the interaction between the fluid and wall particles is calculated. In DPD simulation, fluid particles with a total number of 1932 are bound up within the walls which consists of other 600 particles, and the computational domain is  $V_1 = 14 \times 14 \times 3$  (see Fig. 2).

#### 4 Results and discussion

In order to obtain the relation between density/volume and pressure, fluid particles are bounded up within walls along the x- and y-directions, while the periodic boundary condition is applied in the z-direction. A slice of particles on the right are treated as a rigid piston, as shown in Figs.1 and 2. There are two ways to simulate the response of water to external force. In one way, the system can be first compressed to a relatively smaller volume, and then equilibrated at the constant volume until it achieves a balanced state, during which the pressure can approach to a constant value. After that, the compression and equilibrium processes can be performed repeatedly. The average density, volume and pressure can be obtained at the end of each equilibrium process. In another way, the volume of the system can gradually be decreased at each time step until it reaches the desired volume,

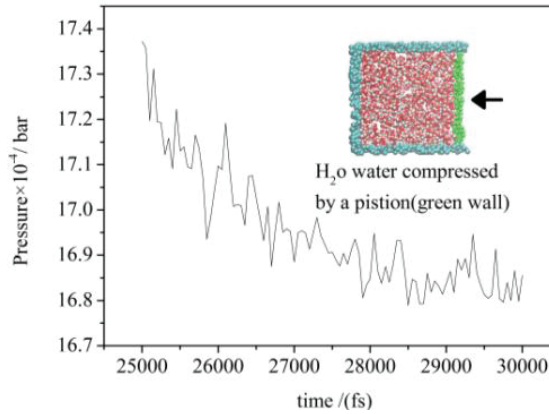


Figure 1: The pressure variation during the equilibrium after compression in MD simulation

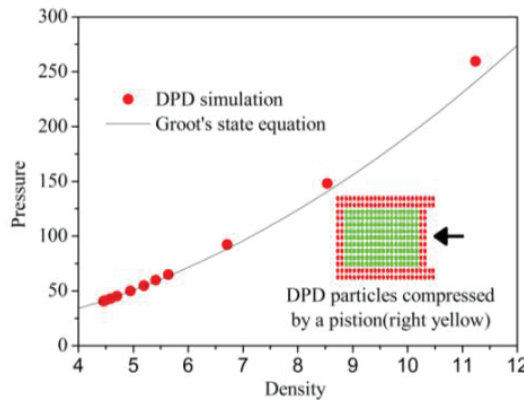


Figure 2: Pressure-density relation for DPD particles during the compression

during which the density, volume and pressure are obtained at the end of every certain number of time steps. In the former way, one of the equilibrium processes in the MD simulation is shown in Fig. 1, from which we can see that the pressure decreases with time and tends towards a constant pressure within a variation of  $\sim 3\%$ . When the fluid is compressed at a given level for a long enough time, the process becomes quasi-static. Hence, the former method is utilized, that is, in both DPD and MD simulations a compressive load is applied incrementally, with a period of equilibrium between two steps, to the piston as shown in Figs. 1 and 2.

In the MD simulations, a computational domain with 200 water molecules (V1 in Tab. 2) was studied first. As illustrated in Fig. 3, the responses of three MD models have the same tendency. The pressure and its gradient are shown to increase with the increase of the absolute value of  $\Delta V/V$ . Figure 4 shows the equilibrium structure of water in MD simulations by plotting the RDF curves. As can be seen, the values of first peaks are the largest, and the magnitude of oscillations become small with time. Similar results can also be found in the DPD simulations.

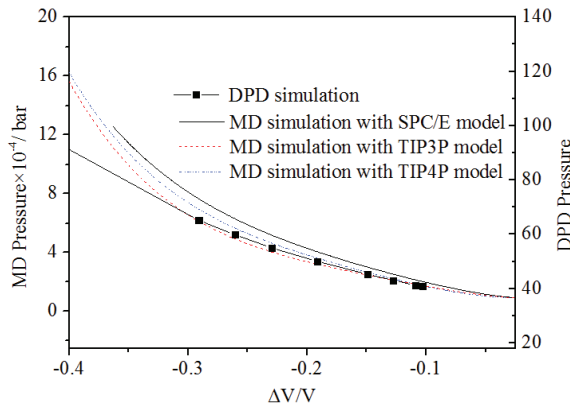


Figure 3: The response to external force of water molecules in MD and particles in DPD

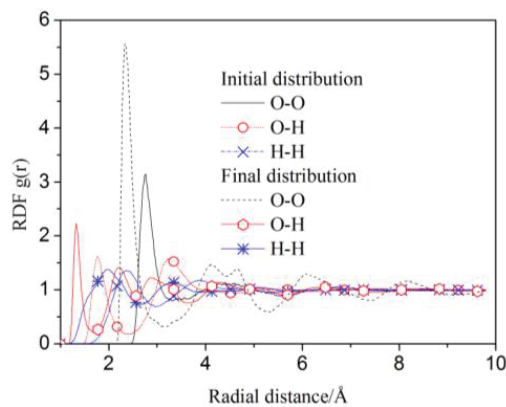


Figure 4: The radial distribution function in MD simulations



Table 2: Different sizes and quantities in MD and DPD simulations

Nos.	type	size	molecules/particles quantity
V1	MD	$31.6 \times 31.6 \times 6 \text{ \AA}^3$	200
V2	MD	$111.8 \times 111.8 \times 6 \text{ \AA}^3$	2509
V3	MD	$223.6 \times 223.6 \times 6 \text{ \AA}^3$	10036
V4	DPD	$14 \times 14 \times 3$	1932
V5	DPD	$50 \times 50 \times 3$	28500
V6	DPD	$100 \times 100 \times 3$	117000

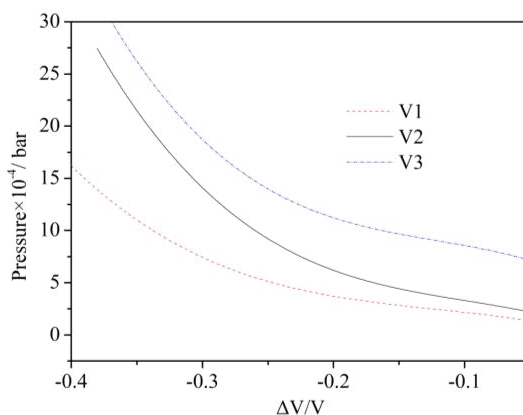


Figure 5: MD pressure-volume relations with different simulation box sizes

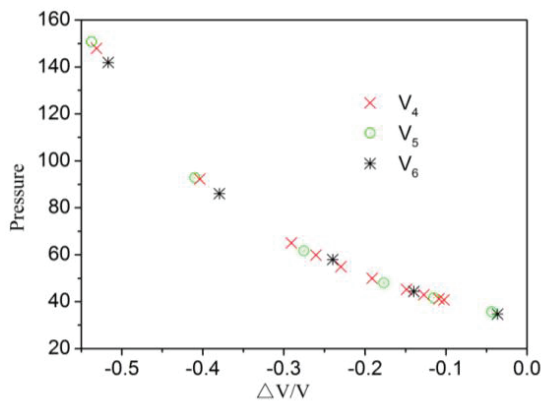


Figure 6: DPD pressure-volume relations with different simulation box sizes

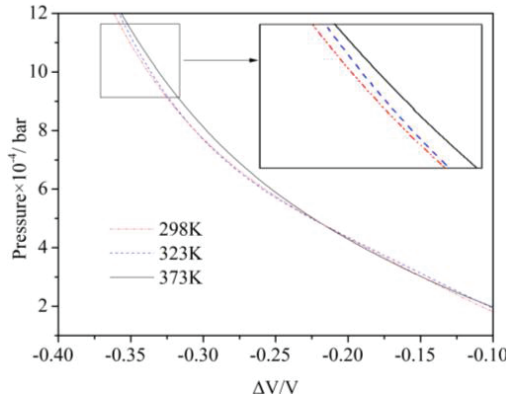


Figure 7: Pressure-volume relations at different temperatures in MD simulations

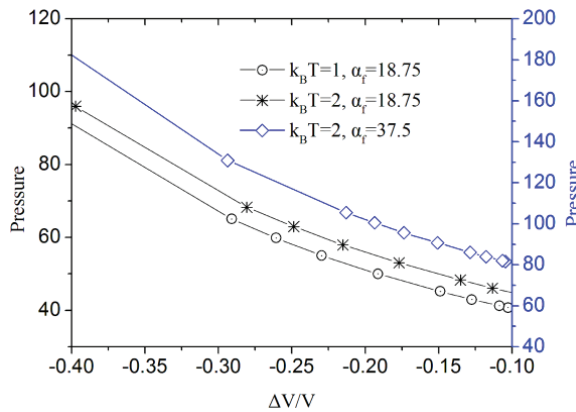


Figure 8: DPD pressure-volume relations at different temperatures

To verify the compressibility of coarse-grained DPD, the pressure-density relation for V4 in Tab. 2 was examined first. As shown in Fig. 2, the data points of pressure calculated for the DPD fluid at different densities are consistent with the curve predicted by Groot’s equation. Although the DPD results demonstrate the same trend as the MD ones within a certain range of  $\Delta V/V$ , the difference between the DPD and MD results become significant with the decrease of volume (increase of pressure), as shown in Fig. 3. The reason might be due to the fact that DPD is a coarse-grained method, in which one DPD particle represents a group of MD molecules. Thus, the DPD fluid particles may show a different performance of physical properties from those in MD, which implies that a scale effect exists.

Besides, the DPD fluid properties depend on the potential functions and other parameters, but the connection between a DPD particle and real material behavior is still unknown for most cases. A better understanding and formulation of the inherent relationship between the MD molecule and DPD particle are therefore required in the future study.

To investigate the size effect, another two computational domains with different sizes and numbers of atoms/particles are considered in MD and DPD simulations as listed in Tab. 2. In the MD simulations, SPC/E water model is employed. As shown in Fig. 5, the water response is significantly different with three box sizes in MD simulations. Although the pressure increases with the decrease of volume for all the three cases, the pressure for V3 is more than twice of that for V1. In DPD simulations, however, the pressure varies in the same trend with the volume change, and there is no size effect on the simulation results.

In both DPD and MD simulations, temperature effect has also been considered. At microscopic scale, the water molecules show almost the same characteristics during the compression at 298K, 323K and 373K, as illustrated in Fig. 7. There is only a small difference during the volume change, and the higher temperature would lead to a higher pressure. In contrast, as shown in Fig. 8 for DPD simulations, the pressure has a relatively large increment from  $k_B T = 1$  to  $k_B T = 2$ , which means that the pressure is sensitive to the temperature. Besides, the increment of the conservative force coefficient also plays an important role on the increase of pressure.

## 5 Conclusions

The MD and DPD simulations have been performed to investigate the water response to external force. In the MD simulations, three molecular water models (SPC/E, TIP3P and TIP4P) show a similar exponential relation between the pressure and volume change, and there are small variations for different temperatures. The DPD simulations illustrate a discrepant trend which is close to a linear relation with either varying temperature or conservative force coefficients. Hence, it is not feasible to relate the DPD results directly to the MD ones. The comparative study indicates that there is a scale effect of the water response to external force between the microscopic scale (MD) and the coarse-grained mesoscale (DPD). The scale effect is caused not only by the coarse-graining and the mapping reliability from MD to DPD, but also by the different interactional potentials at different scales. In addition, the response is dependent on the size of computational domains for MD simulations, but independent to that in DPD ones, implying that there exists a size effect in the atomistic scale simulation. The DPD method appears to be closer to a continuum description of a physical model.

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